Flow of Gas Mixtures through Micro Channel

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Abstract. To investigate flow of gas mixtures through micro channel in detail, the tangential momentum accommodation coefficients of each species for gaseous mixtures were determined by analyzing the Couette flow problem of a slightly rarefied gas between two walls. The molecular dynamics (MD) method for the interaction of gas molecule with the wall surface is combined with the DSMC method for the motion of gas molecules. These obtained accommodation coefficients were applied for the flow of gas mixture through the micro channel as the Maxwell-type boundary conditions, and influence of the surface with adsorbates and the gas concentration on the flow rate of the micro channel was examined. The simulation results show that the velocity slip and the accommodation coefficients for gas mixtures differ from that for a single gas. The differences of the molar concentration of gas mixtures and wall characteristics lead to variations of the flow rate in the channel.

INTRODUCTION

In recent years, remarkable progress has been made in the field of micro-electro-mechanical-systems (MEMS). Therefore, the accurate understanding of the behavior of gas flows in such MEMS is very important due to their numerous industry applications in micro scale technology. Numerical simulation is effective method to predict the fluid flow and evaluate the performance of such micro-devices. However, the conventional continuum method based on the Euler or the Navier-Stokes equations can not be applied for such a gas because of the increase of rarefaction effect, and an approach based on molecular gas dynamics is required for the analysis of such micro-flows. The direct simulation Monte Carlo (DSMC) method of Bird [1] is widely used in molecular gas dynamics and proper technique for calculating the micro-flow [2]. In the DSMC method, a real gas is simulated by a large number of statistically representative particles. The positions, velocities and internal energies of these simulated particles are stored and modified in time in the process of particles motion and interaction with wall. The simplest gas-wall interaction model used in the DSMC calculation is the diffuse reflection. However, the gas-wall interaction is not so simple and sometimes the diffuse reflection is not valid, e.g., at a very clean or high temperature wall, in an ultra vacuum, in a very high speed flow etc. Although the Maxwell-type model and CLL model [3],[4] as the other gas-wall interaction models have been considered, the accommodation coefficient should be specified. In any case, we must estimate accurately the velocity distribution of the reflected molecule at the wall. On the other hand, the molecular dynamics (MD) simulation can predict the trajectory of a molecule as it approaches, interacts with, and scatters from a wall. Many studies have been made using the MD method to analyze the behavior of the reflected molecules [5],[6]. However, as we consider the practical micro channel, the assumption of the interaction between the fluid gas and the wall is required. In previous studies [7],[8], we have studied the rarefied gas flow between two parallel walls by combining the MD method with the DSMC method to investigate effects of the gas-wall interaction on the flow, and it was found that the Maxwell-type boundary condition describes well the distribution function of the reflected molecules. In practice, one deals with gas mixtures more often than with a single gas. Sharipov et al [9] calculated the velocity slip coefficient for binary gaseous mixtures on the basis of the McCormack kinetic model of the Boltzmann equation. However, the velocity slip and the accommodation coefficients are considered to vary with species and wall characteristics. In the present study, therefore, to determine the tangential momentum accommodation coefficients of gas mixtures, the Couette flow of the slightly rarefied gas between two walls is simulated by applied the MD method for the gas-wall interaction and the DSMC

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method for the motion of gas molecules. Moreover, we applied these obtained accommodation coefficients to the simulation of the flow through the micro channel as the Maxwell-type boundary condition, and investigated the influence of the wall characteristics and the gas concentration on the flow rate of the channel.

NUMERICAL METHOD

We consider the Couette flow problem between two walls to obtain the velocity slip and the accommodation coefficient of the wall. The Knudsen number is taken to be 0.2 in the present analysis as a slightly rarefied gas flow. Two types of wall temperatures are selected, 300 K and 600 K. In the present study, the DSMC method is employed in the motions and collisions of gas molecules of the Couette flow. Three types of gases are considered, helium, argon and xenon, and the DSMC simulations of the Couette flow are carried out for the three gas mixtures: helium-xenon, helium-argon and argon-xenon. These gas molecules are assumed to be variable soft sphere (VSS) model [10]. The wall boundary condition is treated as the diffuse reflection.
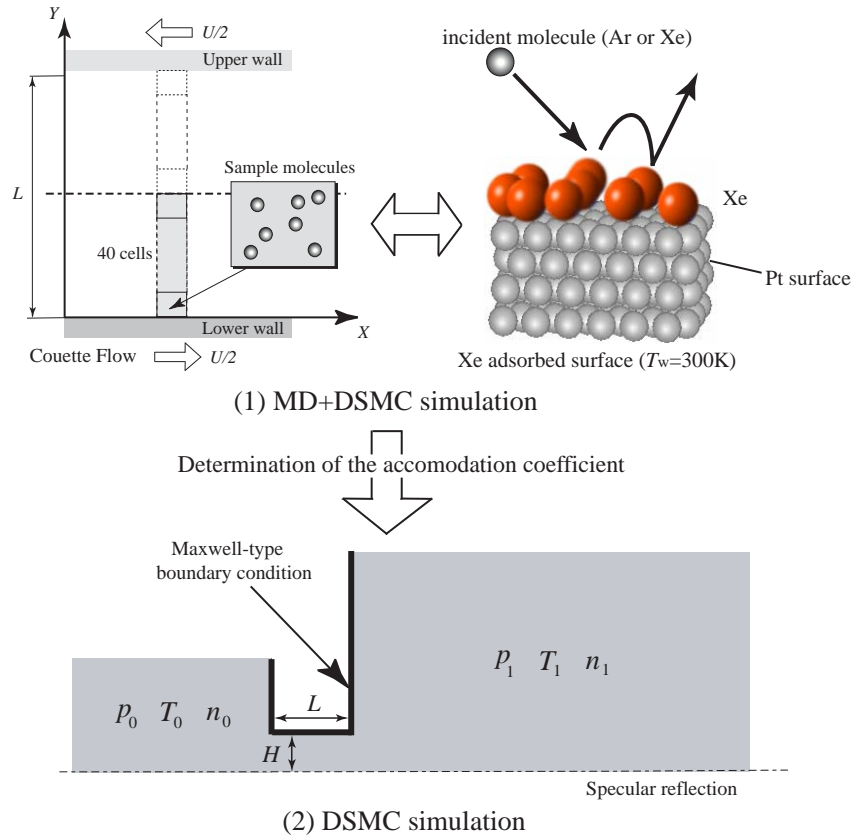

(1) MD+DSMC simulation

(2) DSMC simulation

FIGURE 1. Boundary conditions (1) MD+DSMC simulation of the Couette flow (2) DSMC simulation of the micro channel flow

In the case of gas mixtures simulation of argon and xenon, in order to simulate the gas-wall interaction more accurately, the molecular dynamics method is applied, that is, when a molecule hits the wall surface in the DSMC simulation, we switch to the analysis based on the MD method at this point to trace the motion of the gas molecule, which is going to interact with molecules of the wall (Fig. 1(1)). We assume that the wall consists of a thin platinum layer. The surface of the layer is set on the (111) plane. We take six Pt molecules in the X-direction and another six molecules in the Z-direction on the surface. Four molecular sheets are taken normal to the surface. The periodic condition is applied to the direction parallel to the surface as is usually

assumed in the molecular dynamics. This is a model of a smooth surface. Argon and xenon are taken as the gas molecule in the present MD study. It is found that the argon molecule is not physically adsorbed at the platinum wall surfaces of 300 K and 600 K after interacting with wall molecules. On the other hand, if we take xenon molecule as the gas molecule, the molecule is found to be physically adsorbed on the smooth platinum surface of 300 K and 600 K. Actually, at wall temperature $T_w = 300$ K, nine xenon molecules were adsorbed on one section of the smooth surface consisting of 6×6 Pt molecules parallel to the wall surface, whereas three xenon molecules were adsorbed at 600 K because the kinetic energy of the xenon is increased. The physically adsorbed xenon molecules are moving around on the surface. We shall consider the wall surface with adsorbates at each wall temperature.

As for the interaction potential between molecules, we take the Lennard-Jones potential for Pt-Pt, Xe-Xe, and Ar-Ar interactions. We shall use the Lennard-Jones potential between Xe and Ar whose interaction parameters ϵ and σ are given by the following empirical combining laws [11]. Further, we take the Morse potential for Pt-Xe and Pt-Ar interactions given by [5],[12]. When a gas molecule hits the wall surface in the process of the DSMC simulation, we put the molecule at a distance of 8 σ_{pt} above the most upper Pt molecular layer, where σ_{pt} is the position of minimum Pt potential. The initial velocity of this molecule has been calculated by the DSMC simulation. Newton's equation of motion of molecules are investigated with Verlet's method. The time step of integration is taken to be 1.5×10^{-15}s (argon) and 4.54×10^{-15}s (xenon), respectively. When the gas molecule returns to the position which is more than 8 σ_{pt} away from the wall surface and is not influenced by the wall molecules, we consider that the molecules have been completely reflected, and resume the DSMC calculation there. The molecular dynamics method was applied to trace the motion of all molecules impinging on the wall surface. The computational time required for the typical MD-DSMC simulation is about two hundred hours on the Pentium4 3.2GHz.

The accommodation coefficients obtained from the Couette flow simulation are applied for the gas-wall interaction of the micro channel wall as the Maxwell-type boundary condition. Figure 1(2) shows that the boundary conditions of the micro channel flow simulation. The Knudsen number of the upstream pressure is assumed to be from 5 to 0.05. The ratio of the upstream to the downstream pressure p_0/p_1 is 0.5, and L/H is set to 6 in the present simulation. And we consider two types of wall temperatures, that is, 300 K and 600 K, as well as the Couette flow simulation.

RESULTS AND DISCUSSION

Couette flow

First, we explain the slip coefficient of gas mixture (species 1 and 2) at the wall surface. The asymptotic flow velocity distribution q_x is obtained from the data outside the Knudsen layer, and we can obtain the so-called slip coefficient at the wall surface using this asymptotic distribution. The slip boundary conditions at the wall surface are written as

$$q_x(0) - q_w = \alpha_{12}\lambda\left(\frac{\partial q_x}{\partial Y}\right)_0, \quad \lambda = \frac{\mu v_0}{P_0}, \quad v_0 = \left(\frac{2kT_w}{m_{12}}\right)^{\frac{1}{2}}, \tag{1}$$

where α_{12} is the slip coefficient of gas mixture, q_w the velocity of the wall, λ the mean free path, v_0 the most probable speed, and m_{12} the mean molecular mass of the gas mixture defined as

$$m_{12} = C_{12}m_1 + (1 - C_{12})m_2, \quad C_{12} = \frac{n_1}{n_1 + n_2}, \tag{2}$$

m_1 and m_2 are the molecular mass of species 1 and 2, respectively, n_1 and n_2 are the number density of species 1 and 2, respectively, and C_{12} means the molar concentration. The accommodation coefficients of the tangential momentum σ_1 and σ_2 for species 1 and 2, respectively are defined as

$$\sigma_1 = \frac{\tau_{1i} - \tau_{1r}}{\tau_{1i}}, \quad \sigma_2 = \frac{\tau_{2i} - \tau_{2r}}{\tau_{2i}}, \tag{3}$$

where τ is the tangential momentum, and the subscripts i and r mean the impinging and reflecting molecules, respectively.
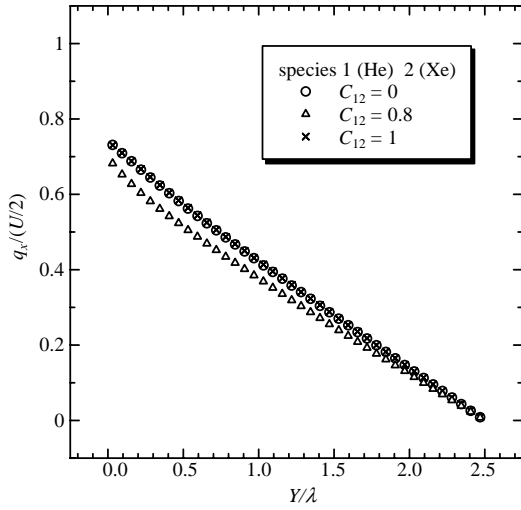
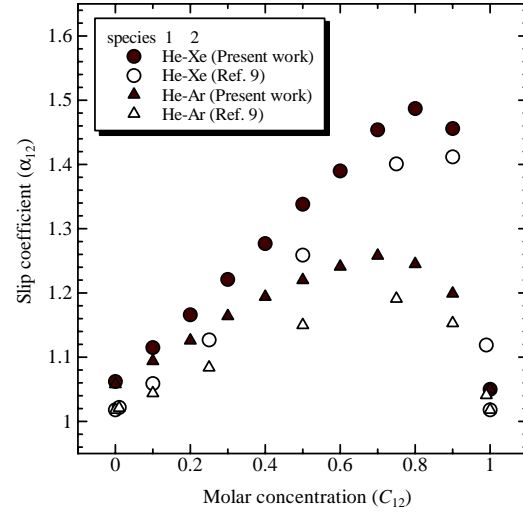**FIGURE 2.** Distributions of flow velocity (diffuse reflection, $T_w = 300K$)

FIGURE 3. Variations of the slip coefficient (α_{12}) with the molar concentration C_{12} (diffuse reflection, $T_w = 300K$)
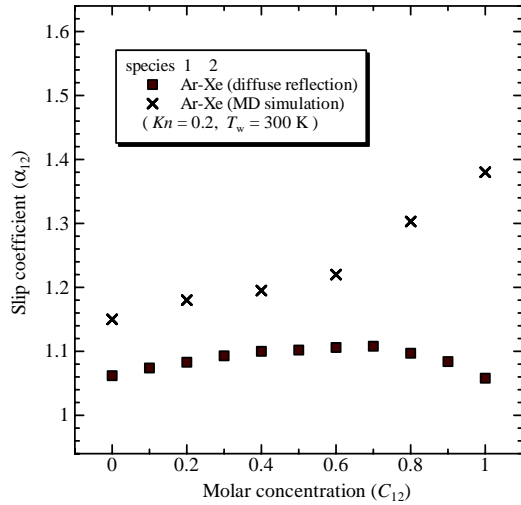

FIGURE 4. Variations of the slip coefficient (α_{12}) with the molar concentration C_{12} (diffuse reflection and MD simulation, $T_w = 300K$)
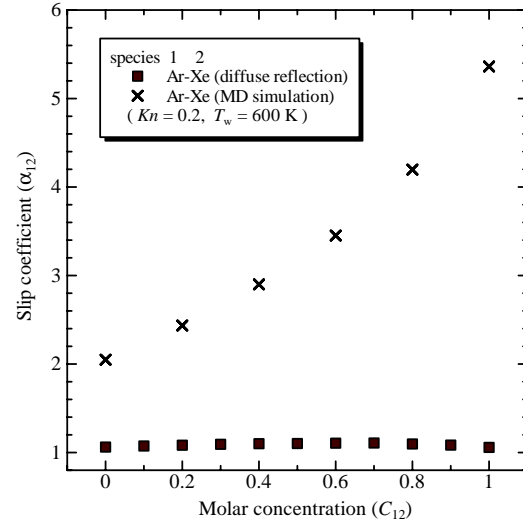

FIGURE 5. Variations of the slip coefficient (α_{12}) with the molar concentration C_{12} (diffuse reflection and MD simulation, $T_w = 600K$)

Figure 2 illustrates the Couette flow velocity distributions of the helium-xenon gas mixture. The lower wall speed $U/2$ is $0.2 \, v_0$, the wall temperature is 300 K and the gas-wall boundary condition is the diffuse reflection. The velocity distributions of a single gas of xenon ($C_{12} = 0$) are identical to that of helium $C_{12} = 1$, whereas, mixture of gases brings about a discrepancy of the velocity distribution. Next, the slip coefficient of gas mixture is calculated from Eq. (1), where the asymptotic line, which goes through the point $Y/\lambda = 2.5$, $q_x = 0$, is obtained by the least squares method using the data of $0.6 < Y/\lambda < 2.5$, that is, we consider that the Knudsen layer extend up to $y \approx 0.6$ from the wall surface. The variation of the slip coefficient (α_{12}) with the concentration C_{12} is shown in Fig. 3, where the wall temperature is 300 K and the gas-wall boundary condition is the diffuse reflection. The value of the slip coefficient increases by mixing gases, and the maximum of the slip coefficient is seen at $C_{12} = 0.7 \sim 0.8$, because a small ratio of heavy species (xenon and argon) influences the slip coefficient more significantly than that of light species (helium). Figures 4 and 5 indicate the comparison of the slip coefficient between two different gas-wall boundary conditions, that is, the diffuse reflection and the MD simulation at $T_w = 300$ K and 600 K, respectively. Since the mass ratio of Ar-Xe is

small, the slip coefficient for the diffuse reflection increases slightly by mixing gases. However, in the case of the MD simulation, the slip coefficient of a single gas changes according to species, and is larger than that of the diffuse reflection. A discrepancy between the diffuse reflection and the MD simulation is larger as the wall temperature is higher. Finally, we have determined the tangential momentum accommodation coefficients from Eq. (4). In the case of the wall temperature $T_w = 300$ K, the accommodation coefficients of argon and xenon are $\sigma_{Ar} = 0.89$ and $\sigma_{Xe} = 0.95$, whereas, at $T_w = 600$ K, $\sigma_{Ar} = 0.41$ and $\sigma_{Xe} = 0.80$, respectively. The simulation results show that the increase of the wall temperature leads to the decent of the accommodation coefficient, especially for the argon molecule.
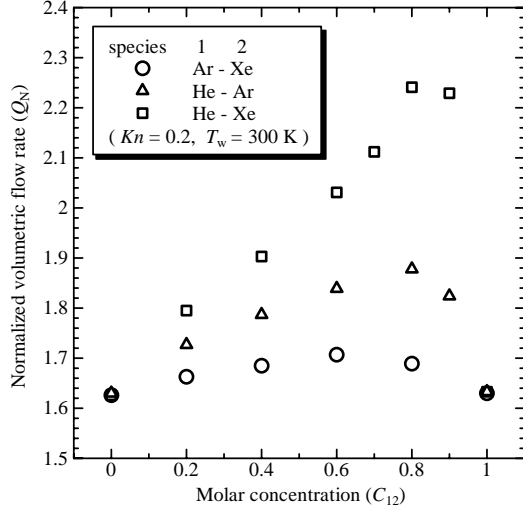

FIGURE 6. Variations of the normalized volumetric flow rate (Q_N) with the concentration C_{12} (diffuse reflection, $T_w = 300$K)
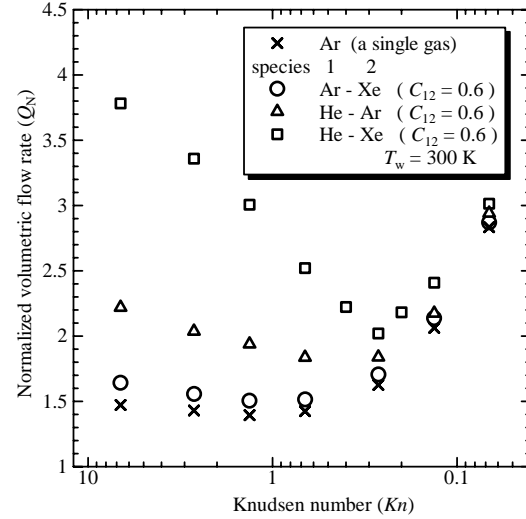

FIGURE 7. Variations of the normalized volumetric flow rate (Q_N) with the Knudsen number (diffuse reflection, $T_w = 300$K)

Micro channel flow

First, the comparison of the volumetric flow rate through the micro channel for various gas mixtures was conducted in the case that the gas-wall boundary condition is assumed to be the diffuse reflection. Figure 6 shows the variations of the normalized volumetric flow rate with the molar concentration C_{12} for various gas mixtures. The normalized volumetric flow rate Q_N is defined by

$$Q_N = \frac{Q_{12}}{\frac{H^2}{2}v_0\left(-\frac{1}{p_m}\frac{\partial p}{\partial x}\right)}, \quad Q_{12} = C_{12}Q_1 + (1 - C_{12})Q_2, \tag{4}$$

where p_m is the pressure at the center of the channel and Q_{12} is the volumetric flow rate of gas mixtures (species 1 and 2). Figure 6 indicates that gas mixing brings about the increase of the normalized volumetric flow rate Q_N. The ratio of this increase is remarkable in the case of the gas mixture of helium-xenon. The value of the maximum of the flow rate is seen at $C_{12} = 0.6$ for argon-xenon, and at $C_{12} = 0.8$ for helium-xenon and helium-argon. Figure 7 shows the relation between the Knudsen number and the normalized volumetric flow rate for a single gas and various gas mixtures. As the flow is rarefied, a difference of the normalized volumetric flow rate between a single gas and gaseous mixtures becomes large. The minimum of the flow rate differs from the species of gas mixture, that is, the location of the minimum moves to the value of smaller Knudsen number as the mass ratio of species is large.

Next, the simulation of the micro channel flow was conducted by applying the tangential momentum accommodation coefficient obtained from the aforementioned Couette flow simulation. The gas-wall boundary conditions is assumed to be the Maxwell-type boundary condition. At the wall temperature $T_w = 300$K, the accommodation coefficients of argon and xenon are close to 1, i.e., $\sigma_{Ar} = 0.89$ and $\sigma_{Ar} = 0.95$, respectively, so the normalized volumetric flow rate is increased slightly. The ascent of the wall temperature brings about the decrease of the number of the adsorbed xenon, and the accommodation coefficient is decreased, especially in the

case of the argon molecule. Consequently, a discrepancy between the diffuse reflection and the Maxwell-type becomes large as the ratio of the argon is increased. The comparison of the volumetric flow rate between the various Knudsen number was illustrated in Fig. 9. In the case of the diffuse reflection, the increase of the wall temperature leads to the slight descent of the flow rate Q_N, whereas, in the case of the Maxwell-type model, as the wall temperature is increased, the flow rate is remarkably increased because the number of the adsorbed xenon is decreased.
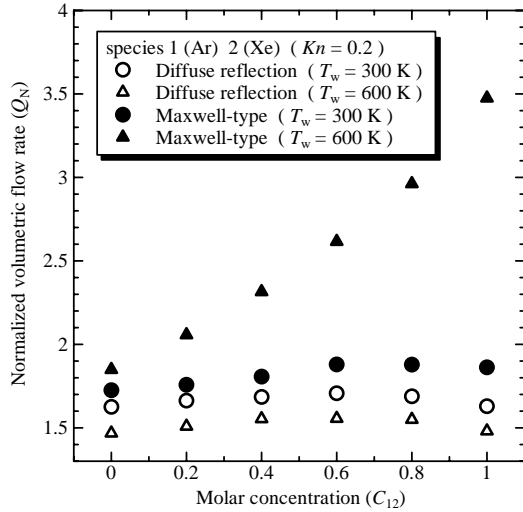

FIGURE 8. Variations of the normalized volumetric flow rate (Q_N) with the concentration C_{12} (diffuse reflection and Maxwell-type model, $Kn=0.2$)
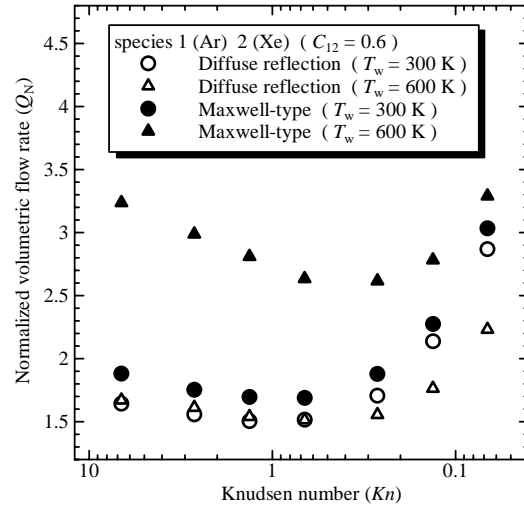

FIGURE 9. Variations of the normalized volumetric flow rate (Q_N) with the concentration C_{12} (diffuse reflection and Maxwell-type model, $C_{12}=0.6$)

CONCLUSIONS

In the present study, we simulated the micro channel flow by using the accommodation coefficient obtained from the Couette flow simulation which is combined the DSMC method with the MD method. The tangential momentum accommodation coefficients of Ar and Xe are 0.89 and 0.95 at $T_w = 300$ K, whereas, 0.41 and 0.80, at $T_w = 600$ K, respectively. These obtained accommodation coefficients were applied for the flow of gas mixture through micro channel as The Maxwell-type boundary condition. The slip coefficient and the normalized volumetric flow rate are increased by mixing gases. In the case of the diffuse reflection, the mass ratio of gas mixture is sensitive for the slip coefficient and the flow rate. The high wall temperature leads to the increase of the normalized volumetric flow rate because of the descent of the adsorbed xenon.

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